A Final Report
Grant No. NAG 1-1050

August 17, 1989 - August 31, 1991

ALGORITHMS FOR FLUIDS CALCULATIONS

Submitted to:

National Aeronautics and Space Administration
Langley Research Center
Hampton, VA 23665-5225

Attention:

Dr. Thomas A. Zang, Jr.
M/S 156

Submitted by:

James M. Ortega
Charles Henderson Professor and
Director, Institute for Parallel Computation

Report No. UVA/528323/CS92/102
August 1991

DEPARTMENT OF COMPUTER SCIENCE

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ENGINEERING
& APPLIED SCIENCE

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This is a final report for NASA Grant NAG-1-1050.

Work leading up to this grant was performed by Professor Ortega and a graduate student, David Harrar, supported by an NSF Fellowship and the NASA Grad-Aero Grant NAG-1-242. Their work, done under the guidance of Dr. T. Zang of NASA-Langley, was concerned with the solution of the three dimensional generalized Poisson equation

$$\nabla(K\nabla u)=f \tag{1}$$

CRAY-2 codes for a SSOR polynomial preconditioned conjugate gradient method were developed and the following papers were published

D. Harrar and J. Ortega, "Optimum m-step SSOR Preconditioning," *J. Appl. Comp. Math.*, 24, 1988, pp. 195-198.

D. Harrar and J. Ortega, "Multicoloring with Lots of Colors," Proceedings of the Third International Conference on Supercomputing, 1989, pp. 1-6.

D. Harrar and J. Ortega, "Solution of Three-Dimensional Generalized Poisson Equations on Vector Computers," *Iterative Methods for Large Linear Systems* (D. Kincaid and L. Hayes, eds.), Academic Press, 1990, pp. 173-191.

Under the present grant, work was continued on this problem in several ways. One of the most promising techniques in the work of Harrar and Ortega was the reduced system conjugate gradient (RSCG) method which arises when one-step SSOR preconditioned conjugate gradient is applied to the red-black ordered equations. Lori Freitag, a Ph.D. student in Applied Mathematics, has continued the development of this algorithm with emphasis on a parallel version suitable for the Intel hypercubes, in particular, the iPSC/860.

Ms. Freitag has made numerous extensions and modifications to the previous CRAY-2 code. The previous code treated only Dirichlet boundary conditions whereas the present one handles combinations of Dirichlet, Neumann and periodic boundary conditions. A consequence of having only periodic and Neumann conditions for (1) is that the coefficient matrix can be singular. We have clarified and extended somewhat the theory of the conjugate gradient method when applied to singular systems. Ms. Freitag has also developed parallel codes for the RSCG method for the Intel iPSC/860. These codes are currently running for a Helmholtz equation in which a term σu is added to (1). This work was helped by Charles Leete, a masters degree student, who during the summer of 1990 at Langley Research Center transferred a previous code by S. Krist to the iPSC/860.

Another project relating to equation (1) was carried out by Robert Falgout, also supported by NASA Grant NAG-1-242. He considered multigrid methods for (1) when the equation is discretized with variable grid spacing. Here, a geometric approach to multigrid is not very satisfactory so he combined the standard geometric approach with the algebraic approach. (In the algebraic approach, the restriction and prolongation operators are defined in terms of the matrix, not the grid.) These algebraic-geometric multigrid methods have advantages in certain situations. Details on this study appear in Mr. Falgout's Ph.D. thesis.

Brett Averick, also supported by NAG-1-242, completed his Ph.D. thesis, which included the development of methods for (1) when K is a function of u so that the problem is nonlinear. In this case, the Jacobian matrix of the corresponding discrete equations is not symmetric

although the skew-symmetric terms are small. We use this fact to approximate the Jacobian by $A(u)$, which is symmetric and positive definite. This gives rise to an approximate Newton method with fast linear convergence, rather than quadratic convergence. The linear systems at each stage are solved approximately by the incomplete Cholesky preconditioned conjugate gradient method with a variable convergence criterion; this allows relatively few conjugate gradient iterations until the iterates are near the solution. Problems on a 63×63×63 grid (250,000 unknowns) are solved on a single processor of the CRAY-2 in 15 - 20 seconds, depending on the initial approximation. A paper on this work by Averick and Ortega will appear in the journal of Applied Numerical Mathematics. Subsequent to the completion of the paper, another very promising approach has been developed based on the formulation of (1) as $\nabla^2\phi(u)=f$. If ϕ is a function such that $\phi'(u)=K(u)$, then

$$\nabla^2\phi(u)=\nabla(\phi'(u)\nabla u)=\nabla(K(u)\nabla u), \tag{2}$$

and (2) is equivalent to (1). Thus, we obtain the solution of (1), in principle, by the two stage process:

I. Solve the Poisson equation

$$\nabla^2 w=f. \tag{3}$$

II. Solve one-dimensional nonlinear equations

$$\phi(u_p)=w_p, \tag{4}$$

where w_p denotes the solution of (4) at a point P in the domain. The equations (4) can all be solved in parallel, and with no communication on a distributed memory machine. Provided that the domain is such that a Fast Poisson Solver can be used for (3), the method is very fast. A paper on this approach is now being prepared for publication. This work was jointly sponsored by NASA Grant NAG-1-1112-FDP.

Narinder Nayer began work during the summer of 1990 on computing eigenvalues of generalized eigenvalue problems involved in stability analysis. One way of proceeding is by converting the generalized problem to a standard eigenvalue problem. There were two approaches here. The first one uses efficient routines (LAPACK) to do the necessary tasks. The second approach was to reorder the problem to reduce the number of operations and then use LAPACK. We were reasonably successful in both these approaches. Using the LAPACK library reduced the time required for the conversion of the generalized problem to the standard problem by approximately a factor of 4. Reordering reduced the time further by a factor 2. Eigenvalue computation is the computer intensive part of the computation. The original code uses the LR method but, since the LR method is a potentially unstable algorithm, we implemented the QR algorithm. However, since the QR method has an operation count of four times the LR algorithm, the time required for calculating all the eigenvalues increases despite using the LAPACK libraries.

We now are in the process of investigating iterative methods for the eigenvalue problem, and computing only a few eigenvalues rather than the whole spectrum. Initially, we have implemented Arnoldi's algorithm which approximates the eigenvalues by building a sequence of Hessenberg matrices. The eigenvalues of these Hessenberg matrices are the approximations to the eigenvalues of the original matrix. To accelerate convergence towards the desired eigenvalues, we use the shift and invert strategy. This process transforms the generalized

eigenvalue problem into a standard one. The code uses the QR implementation of LAPACK to compute the eigenvalues of the Hessenberg matrix. The initial results are encouraging, especially for the larger problem sizes. The speeds can be improved by using the existing LR implementation to calculate the eigenvalues of the Hessenberg matrix. We also plan to compare Arnoldi's algorithm with other algorithms like nonsymmetric Lanczos.

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